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Non-Adiabatic Treatment of Elastic Scattering of Electrons by Atomic Hydrogen

KAZEM OMIDVAR

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January, 1959

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Abstract

The elastic scattering of electrons by atomic hydrogen including the effects of exchange and polarization is calculated. To include the exchange effect the total spin and space function of the incident and the bound electrons is made antisymmetric with respect to interchange of the two electrons. In this way an equation for the wave function of the incident electron similar to the Fock equation is obtained. To include the effect of polarization of the hydrogen atom by the incident electron the wave function for the bound electron is taken in such a way that the electrostatic potential energy between the incident electron and the atom with this wave function becomes equal to the average Coulomb and dipole potential energy of the incident electron, the dipole potential being determined by the experimental value of the polarizability of the hydrogen atom. Since the exchange potential depends on the form of the bound electron wave function, the effect of polarization on the exchange effect is also taken into account. The equation for the wave function of the incident electron is reduced to a set of radial integro-differential equations by the method of partial waves. These equations are integrated numerically using for the bound electron wave function: first, the ground state hydrogenic wave function, and second, the wave function calculated according to the above scheme. The result is that in the second case the calculated curve for the total elastic cross section reproduces most features of the experimental curve for the total elastic scattering cross section of electrons by hydrogen atoms obtained by B. Bederson.

The calculation in the first case has been done by P.M. Morse and W.P. Allis. It seems, however, that there are some errors in their formula. These corrections have been included in the calculated curves.

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I. Introduction

The scattering of electrons by hydrogen atoms has long been used as a model for the scattering of electrons by atomic systems, because it is amenable to some sort of approximate analysis and because it exhibits many of the features of the latter problem. In order that the approximate analysis be useful in the more complicated systems, some basis must be found for evaluating the accuracy of the approximation techniques used in this elementary problem. To that end an extensive series of experiments, involving the elastic scattering of electrons by hydrogen atoms in the range between zero and the first excitation potential of the hydrogen atom , has been undertaken by Professor Benjamin Bederson and his collaborators at New York University[1], and by Dr. Wade L. Fite at General Atomics[2].

Unfortunately, the results of these experiments do not agree with one another, the principal area of disagreement being the fact that Prof. Bederson finds that at about 3 electron volts there seems to be a resonance in the cross section which is of magnitude $100\pi a_0^2$. Fite, at General Atomics, does not find such a peak.

Since the theoretical investigations to date have found no peak, one would think that the Fite results are to be preferred over those of Bederson. The three most important types of calculations which have been done in order to investigate this problem have been a variational calculation[22], and a calculation using a Hartree type of approach including a polarization term[23], and one involving an adiabatic approximation[3]. If the Bederson effect is correct, and a true resonance exists, it may not be surprising that a variational calculation would not uncover it. One would expect that the trial function used in the variational principle would have to resemble the correct wave function to a considerable degree in order for the resonance to appear in this calculation. The ordinary Hartree, or Hartree-Fock method, as applied to this problem, does not, as will be indicated below, accurately describe the polarization of the atom by the incoming electron. In the calculations that have been done using this model, one can correct for this by inserting a phenomenological polarization term into the Hamiltonian. One of the troubles with this method of attack is that the phenomenological polarization term which one inserts must be cut off as one approaches the origin of coordinates, and that the cross section is very sensitive to this cut-off. In the third method[3] the distortion of the atom is accounted for in the adiabatic limit. This calculation leads to an extra potential term representing the effect of the polarized atom on the incident electron and when the incident electron is at large distance from the atom this term approaches the classical value for the potential field due to an induced dipole. The validity of the second order perturbation calculation is based on the assumptions that first, the incident electron moves slowly enough so that, according to the adiabatic principle, the excited states of the hydrogen atom are eigenfunctions of the unperturbed hydrogen atom, and second, that the interaction energy between the incident and the bound electron is small in comparison to the absolute value of the energy of the ground state of the hydrogen atom. The validity of these assumptions, especially the second one, may be questioned since the main contribution to the total cross section is from the region in which the interaction energy between the two electrons is not small in comparison to the absolute value of the energy of the ground state of the hydrogen atom. Thus, the absence of the resonance, when this type of calculation is used, is not necessarily a reason for discarding the experimental results of Professor Bederson.

In this paper, we shall propose a model for the scattering of electrons by hydrogen atoms, which includes an alternative method of taking into account the effects of polarization. It predicts a resonance at approximately the same energy that Bederson found and the cross section is of the same order of magnitude.

We make no claim that our method of including polarization effects is superior to previous attempts. However, when one considers the results obtained in this paper one can see that the theoretical models are still too crude to enable us to distinguish between the two sets of experimental data. Consequently our conclusion must be that the subject is still not exhausted. It is to be emphasized that neither our method nor any of the previous methods which have been used for the analysis of the scattering of electrons by hydrogen atoms can make any estimate of what the errors involved in the calculation are and that consequently the only recourse to the correctness of the method is comparison with the experimental results.

One of the first attempts to analyze this problem has been via a Hartree-Fock calculation, done by Allis and Morse[4]*. The difficulty in choosing a product-type wave function which is characteristic of the Hartree or the Hartree-Fock method, is that no self-consistent procedure is possible once one has made the assumption that a product wave function is to be used. The reason for this is that in order to satisfy the boundary conditions at infinity it is necessary that one of the terms of the product be the ground state hydrogenic wave function. Thus one loses the value of the self-consistent procedure in that one of the terms of the product wave function is now fully determined. However, if one of the product wave functions is the ground state hydrogen atom, then clearly we have not taken into account the effect of the distortion of the atom by the incoming electron. For low energy collisions, this is a serious matter.

---

* There are a few errors in this paper. In the second term of the right-hand side of (5) the factor k^2-E should be k^2+E. This changes the factor k^2-1^a in (8) to k^2+1. Formula (9) should be the same as (8) with the right-hand side multiplied by -1.

We have taken the attitude that it is less important to satisfy the boundary conditions at infinity than it is to describe accurately the effect of the interaction of the incoming electron with the hydrogen atom. We describe the effect of the polarization of the atom by the incoming electron by saying that the effective charge distribution of the atomic system in a static description is given by $e^{-\gamma r}$, where $\gamma < 1$ in atomic units. The effect, then, of the polarization is to spread out the charge distribution of the atomic system. γ is a parameter which is to be determined; it would probably be different for different angular distribution of the incoming electron. It may even be a function of the energy of the incoming electron, although we have not used such a refined model. This effective charge distribution for the bound electron is now substituted in a Hartree, or Hartree-Fock, type of calculation, and the resultant integro-differential equation is integrated numerically on the IBM 704 machine.

If one wished one could satisfy the boundary condition at infinity by changing the effective atomic potential when r_1 is large. We do this by adding to the potential obtained with our charge distribution another, such that the sum is equivalent at this distance to the one obtained when we use the ground state hydrogenic wave function. Since the effective potential for r_1 large is small in any case, it is not expected that this correction would greatly affect our results.

In the following section we discuss the general technique for reducing the three body problem to a one body problem and the way in which one can estimate the value of γ to be used. In Section 3 we derive the equations of motion for the scattered electron on the basis of the model we use. These equations are integrated in Section 4. The results and conclusions are presented in Sections 5 and 6.

2. General considerations

2.1 Reduction of the three-body problem

Any three-body problem can be reduced to a two-body problem by expressing the two independent relative position vectors in terms of the three position vectors. In the present problem, since the mass of the proton is large compared to the mass of the two electrons, the motion of the proton can be disregarded. It is then convenient to take the position of the proton as the origin of the coordinate system. The two relative position vectors would then be the position vectors of the incident and the bound electrons with respect to the proton. We call these vectors $\vec{r}_1$ and $\vec{r}_2$, respectively.

To further reduce the two-body problem to a one-body problem we assume that the total wave function of the incident and the bound electrons is the product of the one-electron wave functions,

$$\psi^{\pm}(\vec{r}_1,\vec{r}_2) = F^{\pm}(\vec{r}_1)\,\phi(r_2) \pm F^{\pm}(\vec{r}_2)\phi(r_1) \ , \tag{2.1}$$

where $\psi^{\pm}(\vec{r}_1,\vec{r}_2)$ is the total wave function and $F^{\pm}(\vec{r}_1)$ and $\phi(r_2)$ are the wave functions of the incident and the bound electrons, respectively. The upper and the lower signs on $F^{\pm}(\vec{r}_1)$ represent the two distinct states of the scattering system in which the two electrons have antiparallel or parallel spins, respectively. The second term on the right-hand side of (2.1) is to make the total spin and space wave function of the scattering system antisymmetric.

By assuming a known form for the bound electron wave function $\phi(r_2)$, the coordinate $\vec{r}_2$ in the equation for the two-body problem can be eliminated by integrating in this equation over coordinate $\vec{r}_2$. The details of this integration will be given in the next section. In this way the three-body problem is reduced to a one-body problem and the resulting equation which depends only upon the coordinate $\vec{r}_1$ describes the scattering of the incident electron.

The choice of $\phi(r_2)$ is, however, important because $\phi(r_2)$ determines the effective interaction between the two electrons; in turn this interaction determines the phase shift and the elastic cross section of the incident electron.

In this paper $\phi(r_2)$ is chosen so that it closely approximates the region of interaction of the two electrons. This choice is based on the following arguments:

From a classical point of view, when the incident electron approaches the hydrogen atom it separates the center of mass of the negative charge distribution from the positive, thereby increasing the energy of the atom. Since this separation is along $\vec{r}_1$, the wave function of the bound electron should have an axis of symmetry in this direction. The wave theory gives, however, a different picture of the charge distribution of the bound electron. This can be understood by expanding the incident electron wave function in terms of the zonal harmonics,

$$F^{\pm}(\vec{r}_1) = \frac{1}{r_1}\sum_{\ell=0}^{\infty} U_\ell^{\pm}(r_1)P_\ell(\mu_1) \quad , \quad \mu_1 = \cos\theta_1. \tag{2.2}$$

It can be seen from this equation that corresponding to each angular momentum quantum number ℓ there is a definite charge distribution of the incident electron. In particular, when $\ell = 0$, the charge distribution of the incident electron is spherically symmetric with respect to the origin. The charge distribution of the incident electron determines, in turn, the charge distribution of the bound electron. In this way we expect that for $\ell = 0$ the charge distribution of the bound electron is spherically symmetric with respect to the origin. For simplification in the wave equation of the incident electron we have assumed that this charge distribution is spherically symmetric for all values of ℓ. Allis and Morse made precisely the same assumptions in their work. The simplest form for such a wave function would be one similar to the wave function of the ground state of the hydrogen atom[5],

$$\phi_0(r) = N_0 e^{-\gamma_0 r} \quad , \quad \gamma_0 = \frac{1}{a_0} \quad , \tag{2.3}$$

N_0 being the normalization constant, and a_0, the Bohr radius. To account for the polarization of the atom, the wave function of the perturbed hydrogen atom is represented by

$$\phi(r) = Ne^{-\gamma r} \tag{2.4}$$

with $\gamma < \gamma_0$. In what follows the relationship between γ and the polarizability of the hydrogen atom through a phenomenological argument is shown.

2.2 Connection between γ and the polarizability

If $\phi(r)$ is to specify the state of the polarized atom it should produce an electrostatic potential which is the sum of the Coulomb and the dipole potentials of such an atom. As far as the relationship between γ and the polarizability is concerned, we can adopt the classical point of view and imagine that the center of mass of the negative charge is displaced a distance d from its unperturbed position in the presence of the electric field of the incident electron. d is connected to the polarizability of the hydrogen atom through the relationship

$$ed = p = \alpha E \qquad , \tag{2.5}$$

where p is the induced electric dipole of the hydrogen atom, α its polarizability, and E the electric field of the incident electron. Since $E = - e/r_1^2$, by (2.5), $d = - \alpha/r_1^2$. When the incident electron is at large distances from the atom a force, due to the induced dipole equal to $2pe/r_1^3 = -2\alpha e^2/r_1^5$, is exerted on the incident electron and this force is derivable from a dipole potential given by

$$V_d = \alpha e/2r_1^4 \ . \tag{2.6}$$

When r_1 is small the main electrostatic interaction between the incident electron and the hydrogen atom is the Coulomb potential of the nucleus given by

$$v_c = e/r_1 \ . \tag{2.7}$$

We can derive an equation which reduces to (2.6) and (2.7) for appropriate values of r_1 by making use of a crude model of the hydrogen atom in an electric field. Assume that when the hydrogen atom is in an electric field, the electronic charge distribution remains spherically symmetric but that its center of mass moves a distance d to the right as is shown in Figure 1. The electric field is due to an electron.

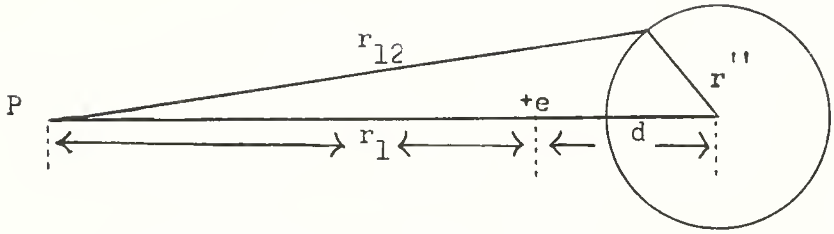

Figure 1

Since the hydrogen atom wave function is given by $\phi(r'') = N_o e^{-\gamma_o r''}$ (see Figure 1), the potential at P due to the electronic charge distribution is given by

$$- e \int \frac{|\phi(r'')|^2}{r_{12}} d\vec{r}'' = - e \int \frac{N_o^2 e^{-2\gamma_o r''}}{r_{12}} d\vec{r}'' .$$

This integral is evaluated in Appendix 1, and by proper substitution we get

$$- e \int \frac{|\phi(r'')|^2}{r_{12}} d\vec{r}'' = e \left(\gamma_o + \frac{1}{r_1+d}\right) e^{-2\gamma_o(r_1+d)} - \frac{e}{r_1+d} .$$

The potential at P, due to both kinds of charges, is then

$$V_P = \frac{e}{r_1} - e \int \frac{|\phi(r'')|^2}{r_{12}} d\vec{r}'' = \frac{e}{r_1} - \frac{e}{r_1+d} + e \left(\gamma_o + \frac{1}{r_1+d}\right) e^{-2\gamma_o(r_1+d)} .$$

The first two terms on the right-hand side represent the potential due to two opposite point charges a distance d apart. Substituting $|d| = \alpha/r_1^2$ in this formula we get

$$V_P = \frac{e}{r_1} - \frac{e}{r_1 + \frac{\alpha}{r_1^2}} + e \left(\gamma_o + \frac{1}{r_1 + \frac{\alpha}{r_1^2}}\right) e^{-2\gamma_o(r_1 + \frac{\alpha}{r_1^2})} .$$

It is seen that the first two terms represent the potential field due to two oppositely charged point particles a distance d apart. The third term is then the effect of spead of the electronic charge (Figure 1). Due to the exponential factor in the third term, the magnitude of this term, when r_1 is either small or large, is much smaller than the difference between the first two terms. If we neglect this term the above equation reduces to

$$(2.8) \qquad V_p = \frac{e}{r_1} - \frac{e}{r_1 + \frac{\alpha}{r_1^2}} = \frac{\alpha e}{r_1(r_1^3+\alpha)} \quad .$$

From this equation we see that for small r_1, $Vp = Vc = e/r_1$ and for large r_1, $V_p = 2V_d = \alpha e/r_1^4$. The fact that V_p is twice the value of V_d instead of being equal to it is due to the way in which we have derived V_p. In this derivation we have assumed that for large r_1, Vp is the dipole potential due to a permanent dipole whose moment happens to be equal to $P = e\ \alpha/r_1^2$, as can be seen from (2.8). Actually in the electric field of an incident electron the hydrogen atom behaves as an induced dipole. A more suitable way to derive (2.8) would be to consider the Coulomb and the induced dipole forces exerted on the incident electron, and to find the potential by calculating the work done by these forces on the incident electron when this electron moves from infinity to the point r_1. However, such a calculation is lengthy and is unduly refined for the crude model from which (2.8) is derived. We are content to write (2.8) in the form

$$(2.9) \qquad V_q = \frac{\alpha e}{r_1(2r_1^3 + \alpha)} \quad .$$

It is seen that V_q reduces to (2.6) and (2.7) for proper ranges of r_1.

Now, by assuming that the perturbed hydrogen atom wave function is given by $\phi(r) = Ne^{-\gamma r}$, the potential field of this atom can be calculated and is given by (Appendix 1)

$$V_\phi = e(\gamma + \frac{1}{r_1})e^{-2\gamma r_1} . \tag{2.10}$$

With two forms of the potential of the incident electron given by (2.9) and (2.10) we require next that the potential energy of the incident electron in its range be the same, using either (2.9) or (2.10). In this way a value for γ is obtained. The main reason for adjusting γ and using (2.10) instead of (2.9) in the equation of motion of the incident electron is to include, through γ, the effect of polarization of the hydrogen atom, in the exchange potential, since γ appears in the expression for this potential. It is this potential that gives rise to a cross section resonance when the incident and the bound electrons have parallel spins. This is discussed in Section 4.

If $F^{\pm}(\vec{r}_1)$ represent the space function of the incident electron, with the upper and lower signs for the total symmetric and antisymmetric space functions respectively, the criterion that the potential energy of the incident electron for the two potential fields be the same is given by

$$e^2 \int \left[\frac{\alpha}{r_1(2r_1^3+\alpha)} - (\gamma + \frac{1}{r_1})e^{-2\gamma r_1} \right] \left| F^{\pm}(\vec{r}_1) \right|^2 d\vec{r}_1 = 0 . \tag{2.11}$$

Substituting the right-hand side of (2.2) into (2.11), and noticing that $P_\ell(\mu)$ are orthogonal functions, we get

$$\sum_{\ell=0}^{\infty} \frac{4\pi e^2}{2\ell+1} \int_0^{\infty} \left[\frac{\alpha}{r_1(2r_1^3+\alpha)} - (\gamma + \frac{1}{r_1})e^{-2\gamma r_1} \right] \left| U_\ell^{\pm}(r_1) \right|^2 dr_1 = 0 . \tag{2.12}$$

This equation is satisfied if we require that

$$(2.13) \qquad \int_0^\infty \left[\frac{\alpha}{r_1(2r_1^3+\alpha)} - (\gamma + \frac{1}{r_1})e^{-2\gamma r_1}\right] \left|U_\ell^\pm(r_1)\right|^2 dr_1 = 0 \,, \qquad \ell = 0,1,2,\ldots \,.$$

The integration of (2.13) would give γ in terms of the polarizability α. It is seen that for each spin and angular momentum state of the incident electron, γ has a different value and, furthermore, since $U_\ell^\pm(r)$ is only known numerically, the solution of (2.13) requires numerical integration. A close inspection of (2.13), however, shows that γ cannot be much different for different states of the incident electron. The reason for this is that when r_1 is very small the sum of the terms in the square bracket approaches a constant and $U_\ell^\pm(r_1)$ behaves like $r_1^{\ell+1}$ (see Appendix III.) The contribution to the integral from this region is therefore negligible. When $U_\ell^\pm(r_1)$ crosses the r_1 axis for the first time in a $U_\ell^\pm(r_1)$ versus r_1 diagram, r_1 is of the order of $\pi/2k_o$ where k_o is the wave number of the incident electron. For small values of k_o, which are of interest in this paper, r_1 is large enough to make each term in the square bracket in (2.13) sufficiently small. We conclude that the largest contribution from each of the two terms in the bracket to the integral (2.13) is from a region in which $U_\ell^\pm(r_1)$ does not change rapidly. We therefore make the approximation that $U_\ell^\pm(r_1)$ is constant in this range and write (2.13) in the form

$$(2.14) \qquad \int_0^\infty \left[\frac{\alpha}{r_1(2r_1^3+\alpha)} - (\gamma + \frac{1}{r_1})e^{-2\gamma r_1}\right] dr_1 = 0 \,.$$

Integral (2.14) is evaluated in Appendix II. The following relationship for γ is found:

$$(2.15) \qquad \gamma = 0.583/\alpha^{1/3} \,.$$

In Figure 2, V_q and V_ϕ, as given by (2.9) and (2.10), are plotted against r for $\alpha = 2.33\ a_o^3$ and its corresponding value of $\gamma = 0.44/a_o$ calculated from (2.15). It is seen that V_q and V_ϕ have the same value at the origin. As r increases V_q becomes larger than V_ϕ for the same r. At approximately $r = 1, V_\phi$ crosses over and becomes larger than V_q. Since V_ϕ vanishes exponentially, V_q becomes larger once more for larger r and remains so for the rest of the range.

2.3 The choice of γ for different angular momentum states of the incident electron

By means of (2.15) the value of γ depends on the polarizability of the hydrogen atom. So far no precise measurement of this polarizability has been made. Even a precise measurement of the polarizability would not give a satisfactory value for γ. The reason for this is that at the classical distance of closest approach of the incident electron the electric field in the vicinity of the hydrogen atom is highly inhomogeneous and its magnitude is far beyond the magnitude of the electric field used to measure polarizability of this atom. The maximum uniform electric field used to measure this polarizability has been 500 e.s.u.[6] while the incident electron at a distance equal to a Bohr radius from the nucleus establishes an electric field at the nucleus equal to $4.8 \times 10^{-10}/(5.29 \times 10^{-9})^2 \cong 1.7 \times 10^7$ e.s.u. Since the formula $p = \alpha E$ is a linear approximation, this method of determining γ is only an approximate one. It is evident, however, that γ depends on the amount of penetration of the incident electron in the potential field of the atom and is therefore related to the classical distance of closest approach.

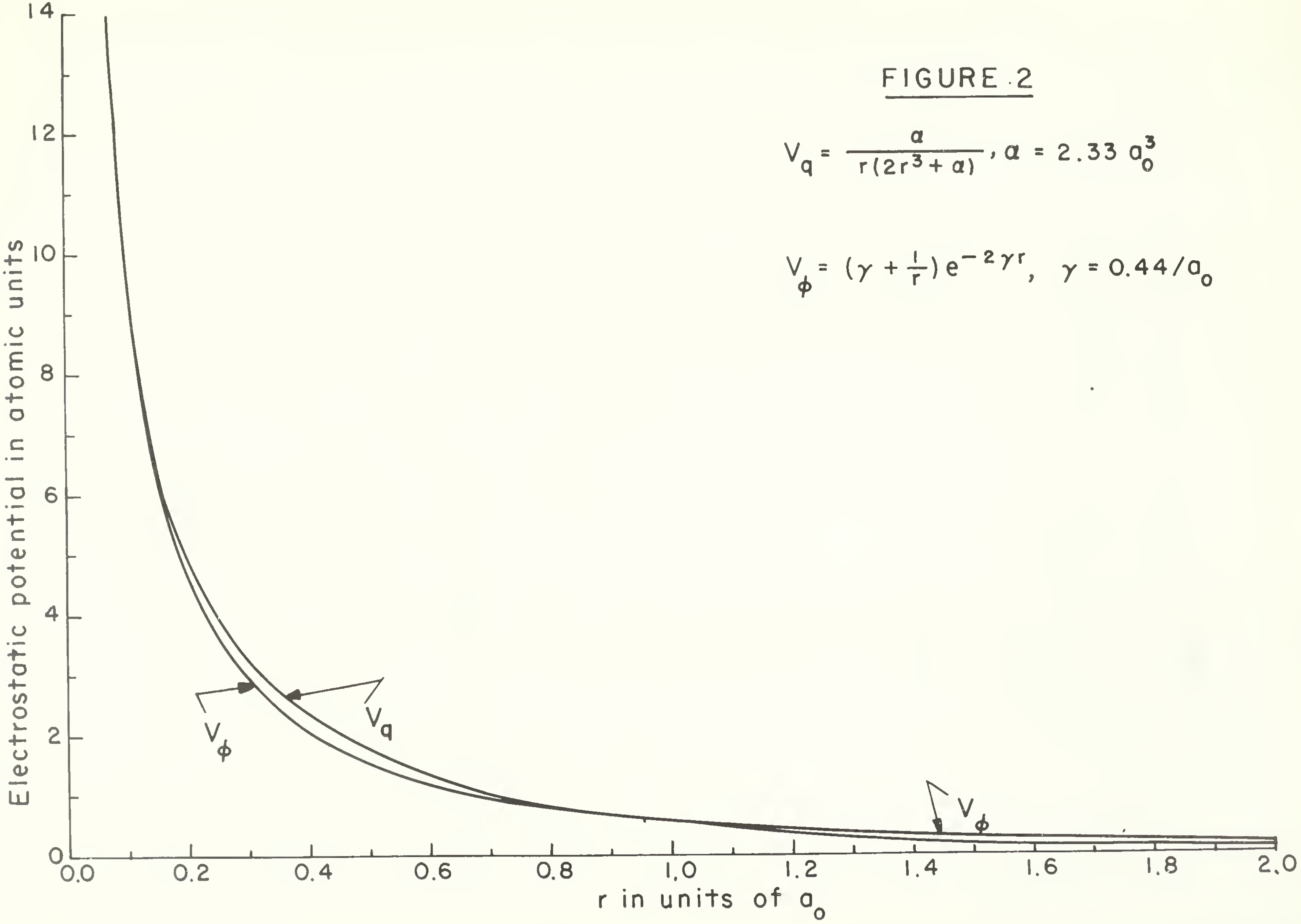

FIGURE 2

$$V_q = \frac{\alpha}{r(2r^3+\alpha)}, \ \alpha = 2.33\ a_o^3$$

$$V_\phi = (\gamma + \frac{1}{r})e^{-2\gamma r}, \quad \gamma = 0.44/a_o$$

This distance is given by

$$(2.16) \qquad d = L/p = \sqrt{\ell(\ell+1)}\,\hbar/\hbar k_o \cong \ell/k_o ,$$

L and p being the angular and linear momentum of the electron. While for small ℓ this distance is of the order of the Bohr radius, its value is different for different ℓ. Hence γ should be different for different angular momentum quantum numbers. The existence of the electrostatic exchange potential as derived in the next section makes the value of γ different for incident electrons with the same angular momentum but different spin states. For a singlet state where the two electrons have antiparallel spins, the exchange potential turns out to be a repulsive one. For a triplet state where the two electrons have parallel spins the opposite situation takes place: the two electrons have a small probability of being close to one another, and this gives rise to a total potential more attractive than the direct potential alone. In this way the exchange potential modifies the total effective potential that the incoming electron sees, and this in turn changes the distance of closest approach of the two electrons with a corresponding change in γ. In the same way it can be inferred from (2.16) that γ depends on k_o. We conclude that γ covers a range of values for different states of the incident electron. In this paper γ is fixed as follows:

As was discussed earlier in this section, the partial wave for the s-scattering is spherically symmetric about the origin, so that on the average the atom is not polarized. We can thus take $\gamma = \gamma_o = 1/a_o$ for s-scattering. With γ fixed for the s-state, it is chosen for the other angular momentum states so that it leads to a value of the total cross section in closest agreement with the experimental results. In this way we find that $\gamma = 0.463/a_o$. We anticipate the results of the numerical integration and mention that with this choice of γ the cross section, due to the states higher than $\ell = 1$, is negligible. By (2.15) $\gamma = 0.463/a_o$ corresponds to $\alpha = 2.00\ a_o^3 = 2.96 \times 10^{-25} cm^3$ according to our model. Sheffers and Stark[7] have measured the polarizability of the hydrogen atom and have found a value equal to $(3 \pm 1) \times 10^{-25} cm^3$ for an electric field intensity of 7×10^4 V/cm. It is seen that the value used in this paper agrees with the experimental value within the limits of the experimental accuracy. The theoretical value for the polarizability, however, is higher. Its value, based on perturbation theory, is $4.50\ a_o^3$ or $6.77 \times 10^{-25}\ cm^3$ [8]. Further discussion of the value of γ is given in Section 5.

3. The wave equation of the incident electron

With a known form of one of the product wave functions, it is possible to obtain the wave equation of the incident electron. The total Hamiltonian of the system of two electrons and one proton is

$$(3.1) \qquad -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{e^2}{r_1} - \frac{e^2}{r_2} + \frac{e^2}{r_{12}} = E$$

where m and e are electronic mass and charge, respectively. $\vec{r}_1$ and $\vec{r}_2$ are position vectors of the incident electron and bound electron, respectively. $r_{12} = |\vec{r}_1 - \vec{r}_2|$. E is the total energy of the system. The total wave function of the two electrons including their spin coordinates should be antisymmetric with respect to the interchange of these electrons in order that this wave function satisfy the Pauli exclusion principle. This condition leads to the symmetric space function for the singlet spin state in which the electrons have antiparallel spins and to the antisymmetric space function for the triplet spin state in which the electrons have parallel spins. The space functions are then of the form

$$(3.2)\qquad \psi^{\pm}(\vec{r}_1,\vec{r}_2) = F^{\pm}(\vec{r}_1)\phi(r_2) \pm F^{\pm}(\vec{r}_2)\phi(r_1)$$

where the upper sign corresponds to the symmetric and the lower sign to the antisymmetric space function, respectively. We introduce a new constant $\gamma_o = 1/a_o = me^2/\hbar^2$ where a_o is the classical Bohr radius and let (3.1) operate on (3.2), obtaining

$$(3.3)\qquad \left[\nabla_1^2 + \nabla_2^2 + 2\gamma_o\left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}\right) + \frac{2m}{\hbar^2}E\right]F^{\pm}(\vec{r}_1)\phi(r_2)$$

$$\pm\left[\nabla_1^2 + \nabla_2^2 + 2\gamma_o\left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}\right) + \frac{2m}{\hbar^2}E\right]F^{\pm}(\vec{r}_2)\phi(r_1) = 0.$$

The wave equation of the incident electron is obtained by multiplying (3.3) by $\phi(r_2)$ and integrating over all coordinates of $\vec{r}_2$,

$$(3.4)\qquad \int \phi(r_2)\left[\nabla_1^2 + \nabla_2^2 + 2\gamma_o\left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}\right) + \frac{2m}{\hbar^2}E\right]F^{\pm}(\vec{r}_1)\phi(r_2)d\vec{r}_2$$

$$\pm\int \phi(r_2)\left[\nabla_1^2 + \nabla_2^2 + 2\gamma_o\left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}}\right) + \frac{2m}{\hbar^2}E\right]F^{\pm}(\vec{r}_2)\phi(r_1)d\vec{r}_2 = 0 .$$

The integration is carried out by noting that $\phi(r) = Ne^{-\gamma r}$. The normalization constant $N = 2\gamma^{3/2}/\sqrt{4\pi}$ is obtained by requiring that $\int \phi^2(r_2)d\vec{r}_2 = 1$. Then the following relationships hold:

$$\nabla^2\phi(r) = N\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}e^{-\gamma r} = \left(\gamma^2 - \frac{2\gamma}{r}\right)\phi(r)$$

$$(3.5)\qquad \left[\nabla^2 + \frac{2\gamma_o}{r}\right]\phi(r) = \left[\gamma^2 + \frac{2(\gamma_o - \gamma)}{r}\right]\phi(r)$$

$$(3.6)\qquad \int \phi(r)\left[\nabla^2 + \frac{2\gamma_o}{r}\right]\phi(r)d\vec{r} = 2\gamma_o\gamma - \gamma^2 .$$

Making use of (3.5) and (3.6) in (3.4) we now have

$$(3.7)\quad \left[\nabla_1^2 + 2\gamma_o\gamma - \gamma^2 + \frac{2m}{\hbar^2}E + 2\gamma_o\int |\phi(r_2)|^2 \left(\frac{1}{r_1} - \frac{1}{r_{12}}\right)d\vec{r}_2\right]F^{\pm}(\vec{r}_1)$$
$$\pm\int \phi(r_2)\left[\nabla_2^2 + \gamma^2 + \frac{2(\gamma_o-\gamma)}{r} + 2\gamma_o\left(\frac{1}{r_2} - \frac{1}{r_{12}}\right) + \frac{2m}{\hbar^2}E\right]F^{\pm}(\vec{r}_2)\phi(r_1)d\vec{r}_2 = 0.$$

Letting k_o, p_o represent the wave number and the momentum of the incident electron at large distances from the atom, respectively, and noting that the energy of the normal state of the hydrogen atom is $-e^2/2a_o = -e^2\gamma_o/2$, we obtain

$$(3.8)\quad k_o^2 = p_o^2/\hbar^2 = 2m(E + e^2\gamma_o/2)/\hbar^2 = 2mE/\hbar^2 + \gamma_o^2\ ,$$

where E is the total energy of the system. Also, by Green's second theorem,

$$(3.9)\quad \int \left[\phi(r_2)\nabla_2^2F^{\pm}(\vec{r}_2) - F^{\pm}(\vec{r}_2)\nabla_2^2\phi(r_2)\right]d\vec{r}_2$$
$$= \int_S \left[\phi(r_2)\frac{\partial}{\partial n}F^{\pm}(\vec{r}_2) - F^{\pm}(\vec{r}_2)\frac{\partial}{\partial n}\phi(r_2)\right]dS\ .$$

The second integral in (3.9) is carried over the surface of a large sphere of radius $r_2 \to \infty$, and since $\phi(r)$ is bounded, this function and its derivative vanish on the surface of this sphere. The surface integral in (3.9) then vanishes and we get

$$(3.10)\quad \int \phi(r_2)\nabla_2^2F^{\pm}(\vec{r}_2)d\vec{r}_2 = \int F^{\pm}(\vec{r}_2)\nabla_2^2\phi(r_2)d\vec{r}_2.$$

Making use of (3.8), (3.10), (3.5) and the result of Appendix I we finally obtain from (3.7):

$$(3.11)\quad \left[\nabla_1^2 + k_o^2 - (\gamma_o - \gamma)^2 + 2\gamma_o\left(\gamma + \frac{1}{r_1}\right)e^{-2\gamma r_1}\right]F^{\pm}(\vec{r}_1)$$
$$\pm\phi(r_1)\int \phi(r_2)\left[k_o^2 + 2\gamma^2 - \gamma_o^2 + \frac{4(\gamma_o-\gamma)}{r}\right]F^{\pm}(\vec{r}_2)d\vec{r}_2 \mp \phi(r_1)\int \phi(r_2)\frac{2\gamma_o}{r_{12}}F^{\pm}(\vec{r}_2)d\vec{r}_2 = 0\ .$$

Equation (3.11), except for the middle term and the third term in the bracket of the first term, is the Hartree Fock equation for the system of two electrons moving in the field of a nucleus [9]. These terms vanish if $\phi(r)$ represents the ground state of the hydrogen atom and if the wave functions of the two electrons can be made orthogonal. The former equation was derived without minimizing the total energy of the system with respect to the two wave functions in contrast to the usual derivation of the Hartree Fock equations.

The three-dimensional equation (3.11) can be reduced to a one-dimensional equation by expanding $F^{\pm}(\vec{r})$ in terms of the zonal harmonics,

$$F^{\pm}(\vec{r}) = \frac{1}{r}\sum_{\ell=0}^{\infty} U_{\ell}^{\pm}(r)P_{\ell}(\mu) \; ; \tag{2.2}$$

$1/r_{12}$ can be expanded in a similar way:

$$\frac{1}{r_{12}} = \frac{1}{r_1}\sum_{n=0}^{\infty}\left(\frac{r_2}{r_1}\right)^n P_n(\mu_{12}) \quad , \qquad r_1 \geq r_2$$

$$= \frac{1}{r_2}\sum_{n=0}^{\infty}\left(\frac{r_1}{r_2}\right)^n P_n(\mu_{12}) \quad , \qquad r_1 \leq r_2$$

$$P_n(\mu_{12}) = P_n(\mu_1)P_n(\mu_2) + 2\sum_{m=1}^{n}\frac{(n-m)!}{(n+m)!}P_n^m(\mu_1)P_n^m(\mu_2)\cos m\,(\phi_1 - \phi_2)$$ [10]

where $\mu_{12} = \cos\theta_{12}$, $\mu_1 = \cos\theta_1$, $\mu_2 = \cos\theta_2$, θ_{12} being the angle between $\vec{r}_1$ and $\vec{r}_2$. θ_1, ϕ_1 and θ_2, ϕ_2 are the spherical coordinates of $\vec{r}_1$ and $\vec{r}_2$, respectively. With the help of these expressions the following equations result:

$$\left[\nabla_1^2 + 2\gamma_0\left(\gamma + \frac{1}{r_1}\right)e^{-2\gamma r_1} + k_0^2 - (\gamma_0-\gamma)^2\right]F^{\pm}(\vec{r}_1)$$

$$= \sum_{\ell=0}^{\infty}\left[\nabla_1^2 + 2\gamma_0\left(\gamma + \frac{1}{r_1}\right)e^{-2\gamma r_1} + k_0^2 - (\gamma_0-\gamma)^2\right]\frac{1}{r_1}\,U_\ell^{\pm}(r_1)P_\ell(\mu_1)$$

$$= \frac{1}{r_1}\sum_{\ell=0}^{\infty}P_\ell(\mu_1)\left[\frac{d^2}{dr_1^2} + 2\gamma_0\left(\gamma + \frac{1}{r_1}\right)e^{-2\gamma r_1} + k_0^2 - (\gamma_0-\gamma)^2 - \frac{\ell(\ell+1)}{r_1^2}\right]U_\ell^{\pm}(r_1)\ ,$$

$$\int \frac{\phi(r_2)F^{\pm}(\vec{r}_2)}{r_{12}}\,d\vec{r}_2$$

$$= \sum_{\ell=0}^{\infty}\sum_{n=0}^{\infty}\Bigg[\int_0^{r_1}\int_{-1}^{+1}\int_0^{2\pi}\phi(r_2)\cdot\frac{U_\ell^{\pm}(r_2)}{r_2}\cdot\frac{r_2^n}{r_1^{n+1}}P_\ell(\mu_2)P_n(\mu_1)P_n(\mu_2)$$

$$+\int_{r_1}^{\infty}\int_{-1}^{+1}\int_0^{2\pi}0(r_2)\,\frac{U_\ell^{\pm}(r_2)}{r_2}\cdot\frac{r_1^n}{r_2^{n+1}}P_\ell(\mu_2)P_n(\mu_1)P_n(\mu_2)\Bigg]r_2^2\,dr_2\,d\mu_2\,d\phi_2$$

$$= \frac{4\pi}{2\ell+1}\sum_{\ell=0}^{\infty}P_\ell(\mu_1)\left[\frac{1}{r_1^{\ell+1}}\int_0^{r_1}\phi(r_2)U_\ell^{\pm}(r_2)r_2^{\ell+1}dr_2 + r_1^{\ell}\int_{r_1}^{\infty}\phi(r_2)U_\ell^{\pm}(r_2)\frac{dr_2}{r_2^{\ell}}\right]\ ,$$

$$\int\phi(r_2)F^{\pm}(\bar{r}_2)d\bar{r}_2 = 4\pi\int_0^{\infty}\phi(r_2)U_0^{\pm}(r_2)r_2\,dr_2\ ,$$

$$\int\frac{\phi(r_2)F^{\pm}(\vec{r}_2)d\vec{r}_2}{r_2} = 4\pi\int_0^{\infty}\phi(r_2)U_0^{\pm}(r_2)dr_2\ .$$

If we substitute the right-hand sides of the last four equations into

(3.11) and equate the coefficients of $P_\ell(\mu_1)$ to zero, the following equations result :

$$\frac{1}{r_1}\left[\frac{d^2}{dr_1^2} + 2\gamma_o(\gamma + \frac{1}{r_1})e^{-2\gamma r_1} - \frac{\ell(\ell+1)}{r_1^2} + k_o^2 - (\gamma_o-\gamma)^2\right]U_\ell^{\pm}(r_1)$$

$$\pm 4\pi\delta_{o\ell}\; O(r_1)\left[(k_o^2 + 2\gamma^2 - \gamma_o^2)\int_o^\infty \phi(r_2)U_\ell^{\pm}(r_2)r_2dr_2 + 4(\gamma_o-\gamma)\int_o^\infty \phi(r_2)U_\ell^{\pm}(r_2)dr_2\right]$$

$$\mp\frac{3\pi\gamma_o}{2\ell+1}\phi(r_1)\left[\frac{1}{r_1^{\ell+1}}\int_o^{r_1}\phi(r_2)U_\ell^{\pm}(r_2)r_2^{\ell+1}dr_2 + r_1^\ell\int_{r_1}^\infty \phi(r_2)U_\ell^{\pm}(r_2)\frac{dr_2}{r_2^\ell}\right] = 0\;.$$

$$\ell = 0,1,2,\ldots.$$

Since $\phi(r) = 2\gamma^{3/2}/\sqrt{4\pi}\, e^{-\gamma r}$, these equations can be written:

$$(3.12)\qquad \left[\frac{d^2}{dr_1^2} + 2\gamma_o(\gamma + \frac{1}{r_1})e^{-2\gamma r_1} - \frac{\ell(\ell+1)}{r_1^2} + k_o^2 - (\gamma_o-\gamma)^2\right]U_\ell^{\pm}(r_1)$$

$$\pm 4\gamma^3\delta_{o\ell}\, r_1 e^{-\gamma r_1}\left[(k_o^2+2\gamma^2-\gamma_o^2)\int_o^\infty e^{-\gamma r_2}U_\ell^{\pm}(r_2)r_2dr_2 + 4(\gamma_o-\gamma)\int_o^\infty e^{-\gamma r_2}U_\ell^{\pm}(r_2)dr_2\right]$$

$$\mp\frac{8\gamma_o\gamma^3}{2\ell+1}e^{-\gamma r_1}\left[\int_o^{r_1}\frac{r_2^{\ell+1}}{r_1^\ell}e^{-\gamma r_2}U_\ell^{\pm}(r_2)dr_2 + \int_{r_1}^\infty \frac{r_1^{\ell+1}}{r_2^\ell}e^{-\gamma r_2}U_\ell^{\pm}(r_2)dr_2\right] = 0\;.$$

$$\ell = 0,1,2,\ldots.$$

The factor $(\gamma_o-\gamma)^2$ appearing in the first term of (3.12) corresponds to the amount of energy that the incident electron has spent in polarizing the hydrogen atom. It owes its existence to the fact that we have not properly included the boundary conditions in our problem, namely that when r_1 approaches infinity the wave function must reduce to an outgoing spherical wave times the ground state hydrogenic wave function. Presumably, if the boundary condition were properly taken into account, such a change of the energy scale would not occur.

Nevertheless, some decision has to be reached about what to do about this term, since for low energies of the incident electron and for $\gamma \neq \gamma_o$, we do not obtain a solution which is outgoing at infinity. For s-scattering we assume that $\gamma=\gamma_o$ and the problem disappears. For higher angular momentum states, when $\gamma \neq \gamma_o$, we can see that effectively the energy of the incoming particle has been reduced to a value equal to $|k_o^2 - (\gamma-\gamma_o)^2|^{1/2}$ instead of k_o. This is correct, the difference being accounted for by the fact that some of the energy of the incoming particle has been used to polarize the atom. If we had a proper model for depolarizing the atom as the incoming particle recedes we would then have the energy reduced again to k_o. Our feeling then is that the term in $\gamma-\gamma_o$ is not one which would persist in a correct model and thus we have eliminated it from the equation. At worst the effect of what we have done is to somewhat distort the energy scale of the incoming particle.

4. Numerical integration of the radial equation

4.1 Method of solution

To facilitate the numerical integration we introduce the following dimensionless variables:

$$(4.1) \qquad x \equiv k_o r_1, \quad x' \equiv k_o r_2, \quad \beta_o \equiv \gamma_o/k_o , \quad \beta \equiv \gamma/k_o .$$

Equations(3.12), with the omission of the factor $(\gamma_o-\gamma)^2$ in the first term and some rearrangements of the limits of inegration, can now be written:

$$(4.2)\qquad \left[\frac{d^2}{dx^2} + 2\beta_o\left(\beta + \frac{1}{x}\right)e^{-2\beta x} - \frac{\ell(\ell+1)}{x^2} + 1\right]U_\ell^{\pm}(x)$$

$$\mp \frac{8\beta_o\beta^3}{2\ell+1}\, e^{-\beta x}\left[\int_0^x \left[\frac{x'^{\,\ell+1}}{x^\ell} - \frac{x^{\ell+1}}{x'^{\,\ell}}\right] e^{-\beta x'}\, U_\ell^{\pm}(x')dx' + C_\ell^{\pm} x^{\ell+1}\right] = 0$$

$$(4.3)\qquad C_\ell^{\pm} \equiv \int_0^\infty \left[x'^{\,-\ell} - \frac{\delta_{0\ell}}{2\beta_o}\left\{(1+2\beta^2-\beta_o^2)x' + 4(\beta_o-\beta)\right\}\right]e^{-\beta x'}\, U_\ell^{\pm}(x')dx'$$

$$\ell = 0,1,2,\ldots$$

Equation (4.3) shows that the values of $C_\ell^{\pm}$ cannot be determined unless the $U_\ell^{\pm}(x)$ are known, and (4.2) shows that the differential equation for $U_\ell^{\pm}(x)$ cannot be integrated unless the $C_\ell^{\pm}$ are known. One way of overcoming this difficulty is to assume some suitable values for $C_\ell^{\pm}$; with these values (4.2) and (4.3) are integrated, and with the new values of the $C_\ell^{\pm}$ the same operation is repeated until consistent values for the $C_\ell^{\pm}$ are obtained. A more suitable method is as follows:

We express $U_\ell^{\pm}(x)$ in terms of the two other functions $U_{\ell_1}^{\pm}(x)$ and $U_{\ell_2}^{\pm}(x)$ such that

$$(4.4)\qquad U_\ell^{\pm}(x) = U_{\ell_1}^{\pm}(x) + C_\ell^{\pm}\, U_{\ell_2}^{\pm}(x) \quad ,$$

where $U_{\ell_1}^{\pm}(x)$ and $U_{\ell_2}^{\pm}(x)$ satisfy the following equations:

$$(4.5)\qquad \left[\frac{d^2}{dx^2} + 2\beta_o\left(\beta + \frac{1}{x}\right)e^{-\beta x} - \frac{\ell(\ell+1)}{x^2} + 1\right]U_{\ell_1}^{\pm}(x)$$

$$\mp \frac{8\beta_o\beta^3}{(2\ell+1)}\, e^{-\beta x}\left[\int_0^x \left[\frac{x'^{\,\ell+1}}{x^\ell} - \frac{x^{\ell+1}}{x'^{\,\ell}}\right] e^{-\beta x'}\, U_{\ell_1}^{\pm}(x')dx'\right] = 0$$

and

$$(4.6)\qquad \left[\frac{d^2}{dx^2} + 2\beta_o\left(\beta + \frac{1}{x}\right)e^{-\beta x} - \frac{\ell(\ell+1)}{x^2} + 1\right]U^{\pm}_{\ell_2}(x)$$

$$\mp \frac{8\beta_o\beta^3}{2\ell+1}\,e^{-\beta x}\left[\int_o^x \left[\frac{x'^{\,\ell+1}}{x^{\ell}} - \frac{x^{\ell+1}}{x'^{\,\ell}}\right]e^{-\beta x'}\,U^{\pm}_{\ell_2}(x')\,dx' + x^{\ell+1}\right] = 0 .$$

If we multiply (4.6) by $C^{\pm}_{\ell}$ and add to (4.5), we obtain (4.2).

The value of $C^{\pm}_{\ell}$ is obtained by substituting (4.4) into (4.3) which gives

$$(4.7)\qquad C^{\pm}_{\ell} = \frac{\displaystyle\int_o^{\infty}\left[x'^{\,-\ell} - \frac{\delta_{o\ell}}{2\beta_o}\left\{(1+2\beta^2-\beta_o^2)x' + 4(\beta_o-\beta)\right\}\right]e^{-\beta x'}\,U^{\pm}_{\ell_1}(x')\,dx'}{1-\displaystyle\int_o^{\infty}\left[x'^{\,-\ell} - \frac{\delta_{o\ell}}{2\beta_o}\left\{(1+2\beta^2-\beta_o^2)x' + 4(\beta_o-\beta)\right\}\right]e^{-\beta x'}\,U^{\pm}_{\ell_2}(x')\,dx'} .$$

For large x, $U^{\pm}_{\ell}(x)$, $U^{\pm}_{\ell_1}(x)$ and $U^{\pm}_{\ell_2}(x)$ are sinusoidal, each with its own amplitude and phase shift. The asymptotic form of (4.4) is then

$$(4.8)\qquad A^{\pm}_{\ell}\sin(x+\delta^{\pm}_{\ell}) = A^{\pm}_{\ell_1}\sin(x+\delta^{\pm}_{\ell_1}) + C^{\pm}_{\ell}A^{\pm}_{\ell_2}\sin(x+\delta^{\pm}_{\ell_2}) .$$

When this equation is expanded we have the identities

$$A^{\pm}_{\ell}\sin\delta^{\pm}_{\ell} = A^{\pm}_{\ell_1}\sin\delta^{\pm}_{\ell_1} + C^{\pm}_{\ell}A^{\pm}_{\ell_2}\sin\delta^{\pm}_{\ell_2}$$

$$A^{\pm}_{\ell}\cos\delta^{\pm}_{\ell} = A^{\pm}_{\ell_1}\cos\delta^{\pm}_{\ell_1} + C^{\pm}_{\ell}A^{\pm}_{\ell_2}\cos\delta^{\pm}_{\ell_2} ,$$

or

$$(4.9)\qquad \tan\delta^{\pm}_{\ell} = \frac{A^{\pm}_{\ell_1}\sin\delta^{\pm}_{\ell_1} + C^{\pm}_{\ell}A^{\pm}_{\ell_2}\sin\delta^{\pm}_{\ell_2}}{A^{\pm}_{\ell_1}\cos\delta^{\pm}_{\ell_1} + C^{\pm}_{\ell}A^{\pm}_{\ell_2}\cos\delta^{\pm}_{\ell_2}} .$$

Equations (4.5) and (4.6) can be integrated from the origin with proper boundary values. $C^{\pm}_{\ell}$ is then calculated* by means of (4.7). Using the asymptotic amplitudes of $U^{\pm}_{\ell_1}(x)$ and $U^{\pm}_{\ell_2}(x)$ together with their phase shifts and the values of $C^{\pm}_{\ell}$, we obtain the phase shifts of $U^{\pm}_{\ell}(x)$ from (4.9). To find the total elastic scattering cross section we note that 3/4 of all the incident electrons have spins parallel to the bound electron spin and the remaining 1/4 have antiparallel spins[11]. The total elastic cross section is then given by[12]

$$(4.10) \qquad S = \frac{4\pi}{k_o^2}\sum_{\ell=o}^{\infty}(2\ell+1)\left[\frac{1}{4}\sin^2\delta^+_\ell + \frac{3}{4}\sin^2\delta^-_\ell\right] .$$

In this paper the numerical integration has been carried out for $\ell = 0,1,2$.

The integration cannot be started without the values of $U^{\pm}_{\ell_1}(x)$ and $U^{\pm}_{\ell_2}(x)$ at the origin. These have been calculated in Appendix III. The results are

$$(4.11) \qquad U^{\pm}_{\ell_1}(x) \underset{x\to o}{=} B^{\pm}_{\ell_1} x^{\ell+1}$$

$$(4.12) \qquad U^{\pm}_{\ell_2}(x) \underset{x\to o}{=} \frac{\pm 8\beta_o\beta^3 x^{\ell+3}}{2(2\ell+1)(2\ell+3)} .$$

The constant $B^{\pm}_{\ell_1}$ in (4.11) is arbitrary. This makes the amplitude of $U^{\pm}_{\ell_1}$ and, through this, the amplitude of $U^{\pm}_{\ell}$ arbitrary at large distances. This is unimportant since we are concerned with the values of the phase shifts of $U^{\pm}_{\ell}$ only. It should be noted that the amplitude of $U^{\pm}_{\ell_2}$ is fixed by (4.12).

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* Actually the integrals appearing in (4.7) are evaluated during the course of integration of (4.5) and (4.6).

4.2 Method of intogration

We use Milne's[13] method to integrate the equations. If a second-order differential equation of the following form is given

$$(4.16)\qquad y'' = f(x,y)$$

the first four points are integrated by means of the Taylor's series to initiate the solution. Then the formula

$$(4.17)\qquad y_{n+1} - 2y_{n-1} + y_{n-3} = 4h^2\left(y''_{n-1} + \frac{1}{3}\,\delta^2 y''_{n-1}\right) + \frac{16}{240}\,h^6 y^{(6)}$$

is used to find y_{n+1}. $\delta^2 y''$ in this formula is defined as

$$(4.18)\qquad \delta^2 y''_n = y''_{n+1} - 2y''_n + y''_{n-1}\ .$$

Since the values of y at the four points x_{n-3}, x_{n-2}, x_{n-1} and x_n are known, (4.17) can be used to find y_{n+1}. As a check on the accuracy of this value the following correction formula is used:

$$(4.19)\qquad y_{n+1} - 2y_n + y_{n-1} = h^2\left(y''_n + \frac{1}{12}\,\delta^2 y''_n\right) - \frac{h^6 y^{(6)}}{240}\ ,$$

to find a more correct value of y_{n+1}. If the difference between the two values is less than a prescribed value for the error of integration, the integration can proceed to the next point.(The interval of integration can even be doubled to accelerate the integration.) But if the difference is more than a prescribed value the interval is halved and the integration is repeated until the desired accuracy is attained. From (4.17) and (4.19) this difference is $17h^6 \cdot y^{(6)}/240$.

The integrals appearing in (4.5) and (4.6) can be integrated from the origin while the integration of the equations is progressing. Simpson's rule[14] is used for evaluation of the integrals. If $y = \int_{x_0}^{x_2} y'(x)dx$, then according to this rule

$$(4.20) \qquad y_2 - y_o = \frac{h}{3}(y'_o + 4y'_1 + y'_2) - \frac{h^5 y^{(5)}}{90} .$$

This rule is not only accurate but simple because a knowledge of only one previous value of the integral is required to continue the integration.

Equations (4.5) and (4.6) were integrated on the IBM 704 digital computer.

5. Interpretation of the results and comparison with experiment

As was pointed out in Section 2, the choice of $\gamma = 1.00/a_o$ for s-scattering and $\gamma = 0.463/a_o$ for higher angular momentum scattering would lead to a total elastic cross section in close agreement with the experiment. The reason for taking $\gamma = 1.00/a_o$ for s-scattering is that the s-partial wave is spherically symmetric about the origin, and polarization of the atom can be neglected. There are other reasons for this assumption.

The s-scattering cross section at $k_o = 0$ increases with a decrease in γ according to the formula

$$(5.1) \qquad S(k_o = 0) = 4\pi a^2 \sim 1/\gamma^2 ,$$

S being the s-scattering cross section and a the scattering length[15]. For intermediate values of k_o the largest contribution to the phase shift is from the Coulomb potential, and polarization does not play an important role while in other angular momentum states the Coulomb potential is effectively screened by the "centrifugal potential" and the effect of the polarization potential is more evident[16]*. These considerations show that the only important effect of taking γ less than 1 in the s-state is to increase the total cross section at $k_o = 0$. Since Bederson's experimental curve does not extend to $k_o=0$, we cannot determine γ in this case by comparing our results with the experimental ones. However, the calculated cross section according to the present model with $\gamma = 1/a_o$ agrees with the independent calculations of the elastic scattering cross section of electrons by hydrogen atoms at $k_o=0$[17],[18]. We have therefore adopted the value of $\gamma = \gamma_o$ for s-scattering in this paper. For other angular momentum states it is found that $\gamma = 0.463/a_o$ gives rise to a curve for the total cross section in close agreement with the experimental curve of B. Bederson.

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* Similar conclusions are reached with the model used in [3], Section 3.

With this value for γ the angular momentum states higher than $\ell = 1$ do not contribute appreciably to the cross section. For example, the d-state has a maximum cross section about $2\pi a_o^2$ when $k_o = 0.7/a_o$. For this reason the contribution of angular momentum states higher than $\ell = 1$ are neglected.

In the following pages the results of the numerical integration are tabulated and are shown, graphically.

In Table 1 are the numerical values of the phase shifts and the scattering cross sections when the incident electron is in each possible spin and angular momentum state, and for $\gamma = 1.00$. In Table II the same results are given for $\gamma = 0.463$ for p-states.

Figure 4 shows the phase shifts as a function of the incident electron energy for the 2 p-states considered in this paper. It is seen that the singlet phase shift assumes negative values for some range of the incident electron energy. This is explained by the fact that in the singlet state the two electrons have some affinity for each other. This affinity is expressed by a positive electrostatic exchange potential energy as is seen by the lower sign in (3.11). This potential energy may be large enough

Table I

Elastic Scattering of Electrons by Hydrogen Atoms

Solution of the Hartree Fock Equation with H-Wave Function $\Phi_o(r) = Ne^{-\gamma r}$

δ: Phase Shift in Radians; S: Cross Section in Units of πa_o^2

k_o: Wave Number in a.u. E: Incident Electron Energy in eV

$\gamma = 1.00$

k_o	E	$\ell = 0$ Singlet		$\ell = 0$ Triplet		$\ell = 1$ Singlet		$\ell = 1$ Triplet		Total Cross Section
		δ	S	δ	S	δ	S	δ	S	
0.00	0.00									
0.01	0.00136	3.0606	65.52	3.1181	16.51					82.0
0.10	0.136	2.395	46.1	2.908	16.1	-0.001	0.001	0.002	0.005	62.2
0.20	0.544	1.870	22.83	2.679	14.93	-0.009	0.005	0.017	0.062	37.8
0.30	1.224	1.508	11.1	2.461	13.2	-0.024	0.020	0.052	0.273	24.6
0.40	2.176	1.239	5.588	2.257	11.22	-0.046	0.040	0.105	0.618	17.5
0.50	3.400	1.031	2.94	2.070	9.25	-0.071	0.060	0.172	1.05	13.3
0.60	4.896	0.869	1.620	1.901	7.459	-0.092	0.071	0.232	1.323	10.5
0.70	6.664	0.744	0.936	1.749	5.93	-0.109	0.072	0.286	1.46	8.40
0.80	8.704	0.651	0.574	1.614	4.679	-0.116	0.062	0.321	1.398	6.71
0.90	11.02									
1.00	13.6									

Table II

k_o	E	$\ell = 0$ Singlet		$\ell = 0$ Triplet		$\ell = 1$ Singlet		$\ell = 1$ Triplet		Total Cross Section
		δ	S	δ	S	δ	S	δ	S	
0.00	0.00	3.142		3.142						
0.01	0.00136	3.061	65.5	3.118	16.5					82.0
0.10	0.136	2.395	46.1	2.908	16.1	-0.020	0.125	0.076	5.24	67.6
0.20	0.544	1.870	22.8	2.679	14.9	-0.105	0.819	0.521	55.7	94.2
0.25	0.850					-0.156	1.15	0.759	68.2	100.4*
0.30	1.22	1.508	11.1	2.461	13.2	-0.200	1.31	0.895	60.9	86.5
0.40	2.18	1.239	5.59	2.257	11.2	-0.243	1.09	0.963	37.9	55.8
0.50	3.40	1.031	2.94	2.070	9.25	-0.208	0.513	0.933	23.2	35.9
0.60	4.90	0.869	1.62	1.901	7.46	-0.105	0.091	0.885	15.0	24.2
0.70	6.66	0.744	0.936	1.749	5.93	0.032	0.006	0.839	10.2	17.1
0.80	8.70	0.651	0.574	1.614	4.68	0.164	0.125	0.800	7.24	12.6
0.90	11.0									
1.00	13.6									

Elastic Scattering of Electrons by Hydrogen Atoms

Solution of the Hartree Fock Equation with H-Wave Function $\Phi_o(r) = Ne^{-\gamma r}$

γ = 1.00 for s-scattering

γ = 0.463 for p-scattering

k_o: Wave number of the incident electron in a.u.

E: Energy of the incident electron in e.v.

δ: Phase shift in radians

S: Elastic cross section in πa_o^2 units.

* s-scattering cross section by interpolation

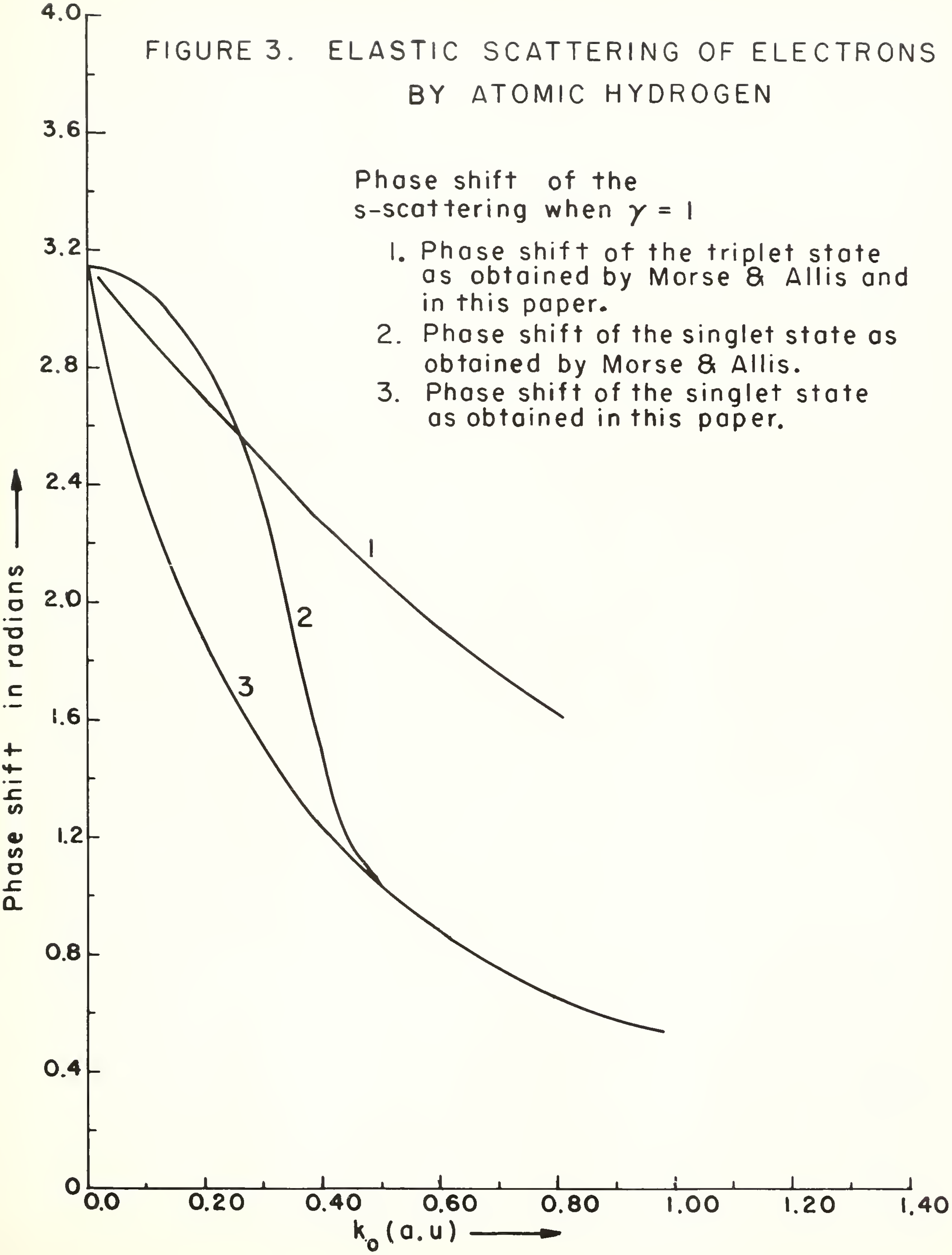

FIGURE 3. ELASTIC SCATTERING OF ELECTRONS BY ATOMIC HYDROGEN

Phase shift of the s-scattering when $\gamma = 1$

1. Phase shift of the triplet state as obtained by Morse & Allis and in this paper.
2. Phase shift of the singlet state as obtained by Morse & Allis.
3. Phase shift of the singlet state as obtained in this paper.

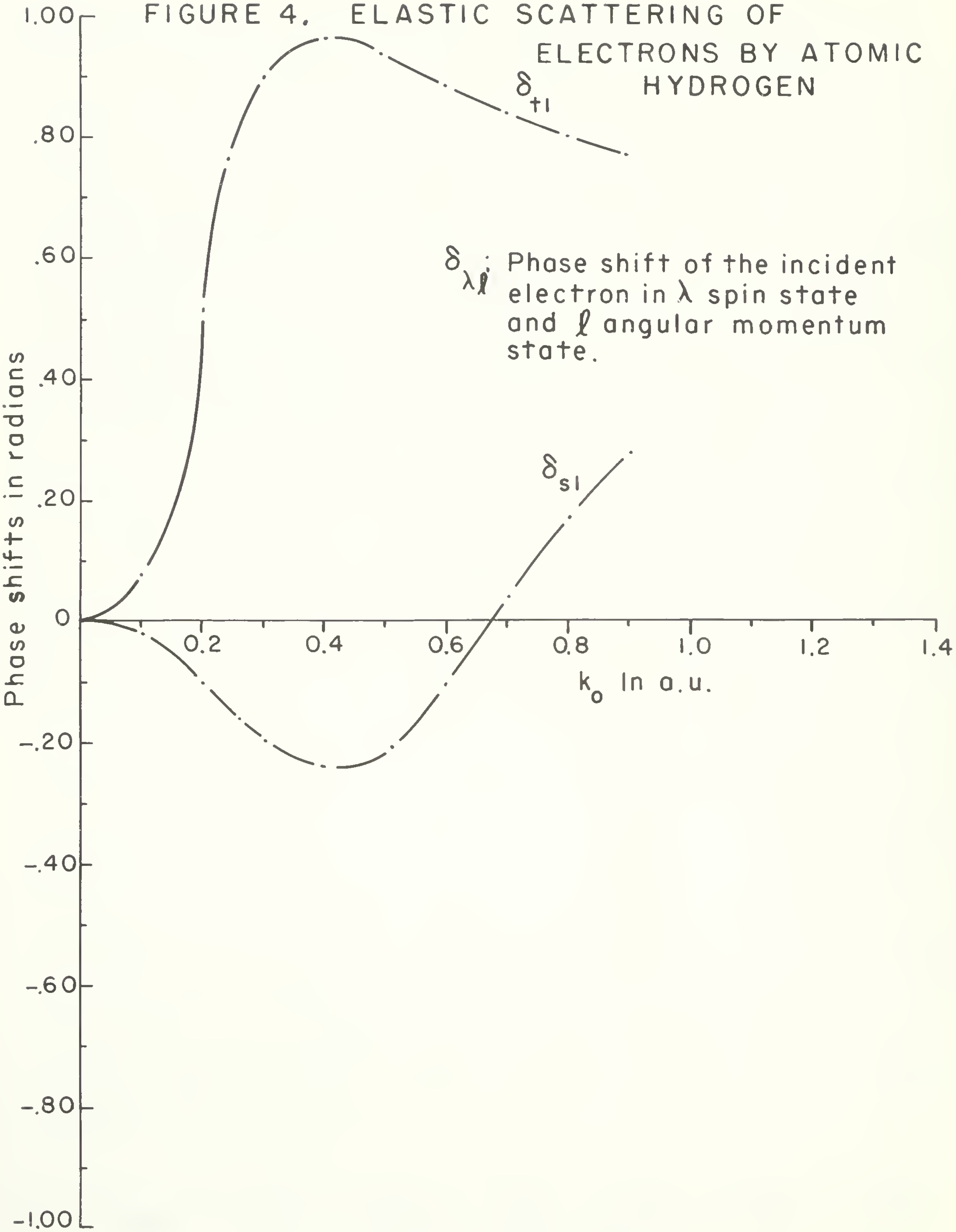

FIGURE 4. ELASTIC SCATTERING OF ELECTRONS BY ATOMIC HYDROGEN

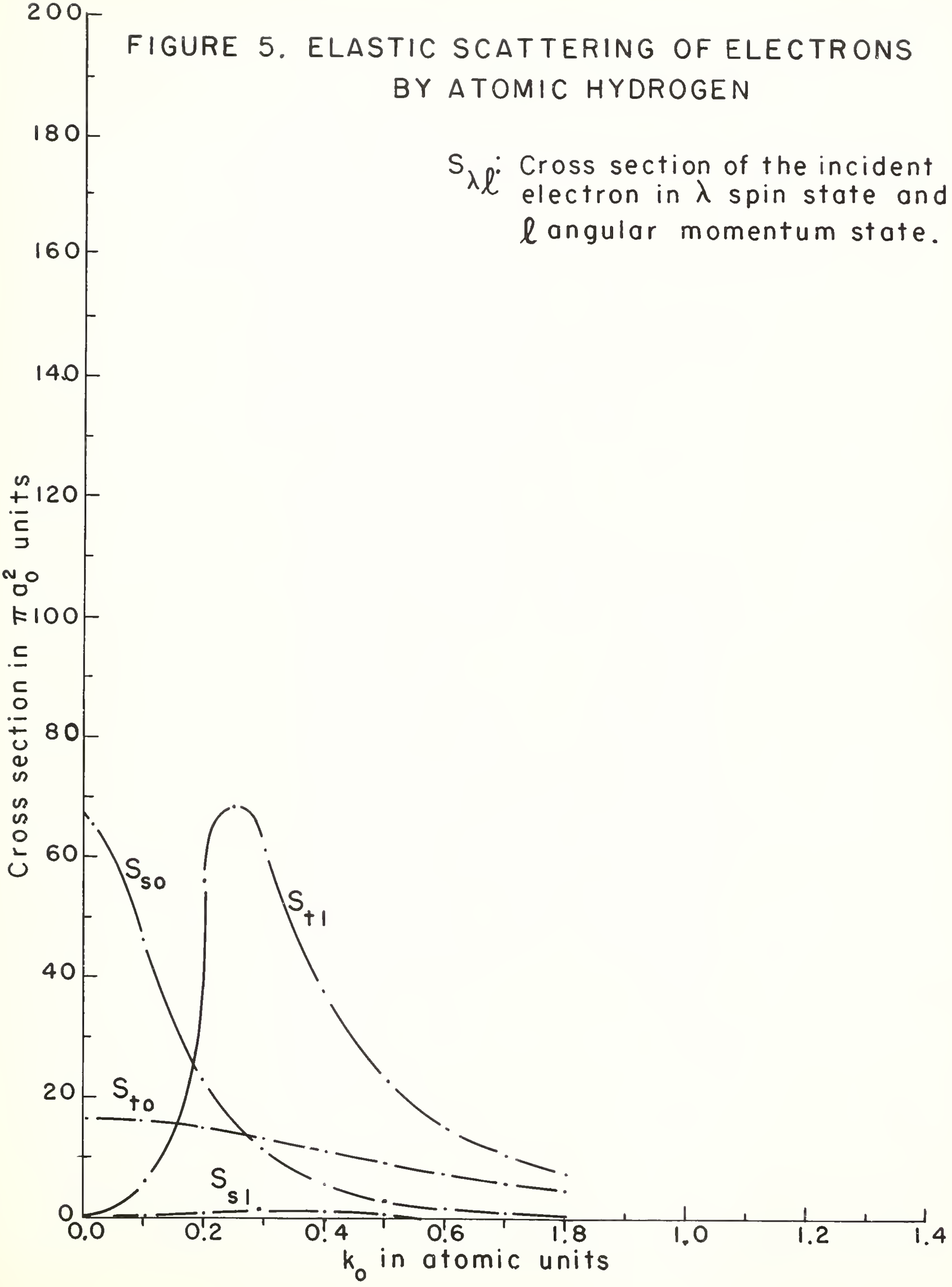

FIGURE 5. ELASTIC SCATTERING OF ELECTRONS BY ATOMIC HYDROGEN

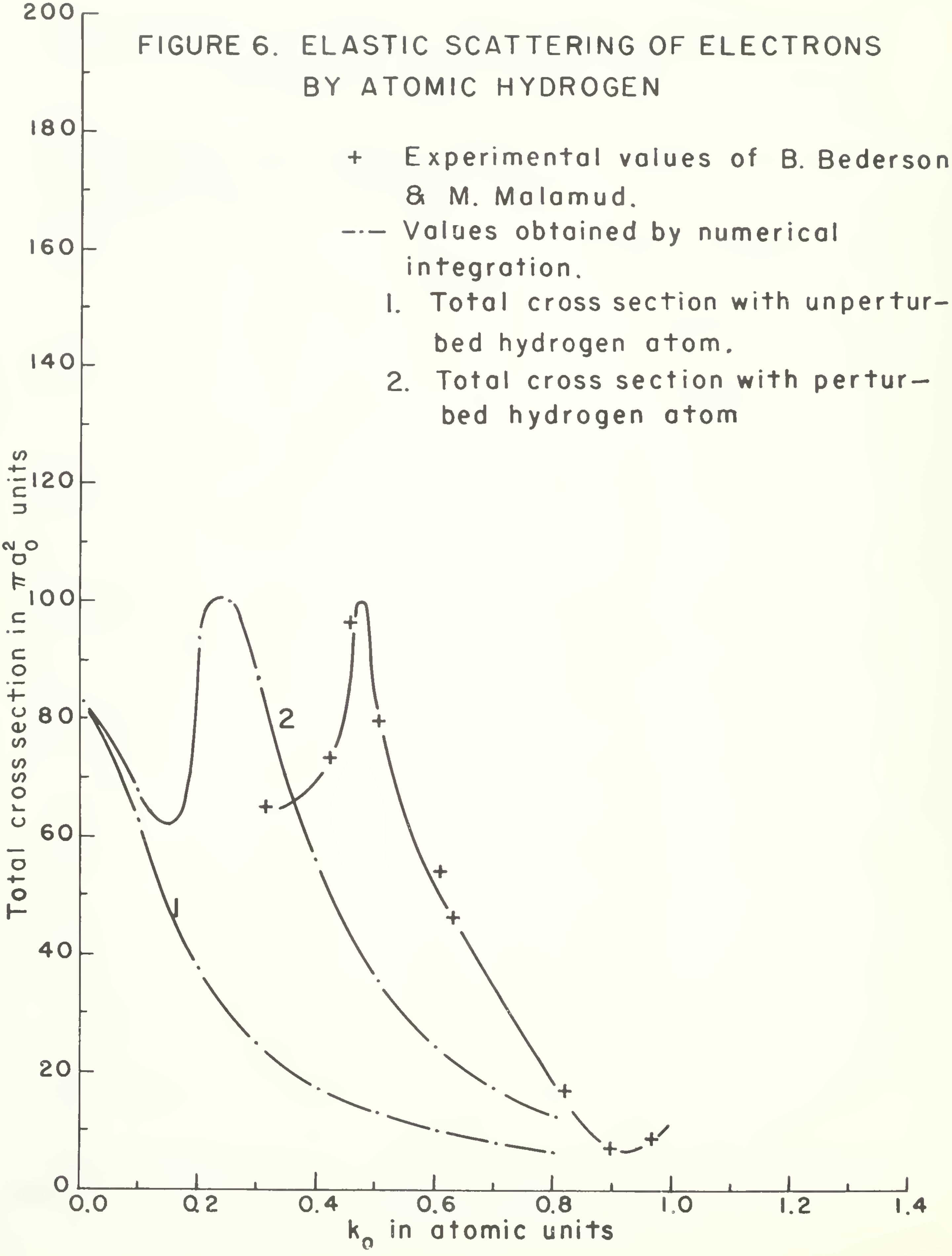

FIGURE 6. ELASTIC SCATTERING OF ELECTRONS BY ATOMIC HYDROGEN

to outweigh the attractive direct potential energy. The zero phase shift signifies that the average exchange potential completely balances the average direct potential.

The phase shifts for the triplet states, on the other hand, are always positive due to the fact that the exchange potential in these states is always attractive and adds to the effect of the direct potential.

In Figure 5 the contribution to the total cross section from each state is shown graphically. It is seen that the largest contribution comes from the triplet state with $\ell = 1$.

In Figure 6 the total cross section is shown for $\gamma = 1.00$ in the s and p-states (curve 1); and for $\gamma = 1.00$ in the s-state and $\gamma = 0.463$ in the p-state (curve 2). The experimental curve of B. Bederson is also redrawn for comparison. It is seen that when γ changes from 1.00 to 0.463 in the p-state, the theoretical curve reproduces most of the features of the experimental curve. As shown in Section 2, a value of $\gamma = 0.463$ corresponds approximately to a value for the polarizability of the hydrogen atom equal to 2.00 a_o^3 or 2.96×10^{-25} cm^3. Sheffers and Stark[7] have measured polarizability of the hydrogen atom and have found a value equal to $(3 \pm 1) \times 10^{-25}$cm^3 for an electric field of 7×10^4v/cm. It is seen that the value used in this paper agrees with the experimental value within the limits of the experimental accuracy.

Figure 3 is the comparison of the s-scattering phase shift for $\gamma = 1.00$ as obtained in this paper and as calculated by Morse and Allis[4]. There are some discrepancies for singlet scattering due to the errors pointed out in page 3. This discrepancy may explain most of the differences for the singlet state between the curve obtained by a variational method by Massey and Moisewitsch[19] and the curve obtained by numerical integration by Morse and Allis.

. . . .

It should be noted that a better agreement with the experimental curve can be obtained if contribution to the total cross section by higher angular momentum states with different γ is taken into account. These values for γ should be less than 0.463. As ℓ increases, the classical distance of closest approach increases and the incident electrons with lower values of k_o do not enter the potential field of the atom. As a result the maximum contribution to the cross section appears at higher values of k_o. In this way a theoretical curve in better agreement with the experimental curve can be obtained. We have not carried out this program here principally because there is no unique way of finding the values of γ for each state.

We also enumerate the other approximations used in the present static model which may be partly responsible for the discrepancy between the theory and the experiment.

1. The charge distribution of the bound electron depends on the position vector $\vec{r}_1$ of the incident electron. In the assumed model this charge distribution is independent of $\vec{r}_1$ and is a function of $|\vec{r}_2|$ only.

2. While the perturbed hydrogen atom wave function is spherically symmetric with respect to the origin in s-scattering, it has a different symmetry in higher angular momentum scattering. We have assumed that this wave function is spherically symmetric in all states.

3. The neglect of the term $(\gamma_0-\gamma)^2$ in (3.12) has the effect of distorting the energy scale in some unknown way.

4. A less important approximation was used in the derivation of (2.14) from (2.11) by assuming that the radial wave functions do not change rapidly in the course of integration.

5. The total wave function is given only approximately as a symmetrized product of one-electron wave functions.

6. Conclusion

By making some reasonable assumptions in the scattering of electrons by hydrogen atoms it was shown that the essential features of the experimental results of B. Bederson can be reproduced as is shown in Figure 6, Section 5. The discrepancy between the two curves is thought to be due to the approximations made in the assumed model. These approximations are enumerated at the end of Section 5. The resonance in the elastic cross section of electrons by hydrogen atoms at about 3 ev incident electron energy, as described by B. Bederson, is believed to be due to a triplet state. The largest contribution to the resonance in this state comes from $\ell = 1$ although higher angular momentum may also be effective.

The model outlined in this paper has not the superiority of a model in which the bound electron wave function changes continuously with the position vector $\vec{r}_1$ of the incident electron but this disadvantage is outweighed by its simplicity. This model can be extended to the scattering of electrons by any atom, provided the potential field of the atom is defined.

Appendix I

The potential due to the wave function $\phi(r)$ is readily obtained by making use of the Gauss' theorem. The charge density of the bound electron is $-e|\phi(r_2)|^2 = -eN^2e^{-2\gamma r_2}$. The contribution to the potential of the incident electron from all negative point charges in space for which $r_1 > r_2$ is the same as the contribution from all these charges placed at the center of the coordinate system. The contribution to the potential from all point charges for which $r_1 < r_2$ would not change if the incident electron were placed at the origin. From these considerations the following results are obtained:

$$-e\int\frac{|\phi(r_2)|^2}{r_{12}}d\vec{r}_2 = -4\pi eN^2(\frac{1}{r_1})\int_0^{r_1}e^{-2\gamma r_2}r_2^2dr_2-4\pi eN^2\int_{r_1}^{\infty}e^{-2\gamma r_2}(\frac{1}{r_2})r_2^2dr_2$$

$$= e(\gamma+\frac{1}{r_1})e^{-2\gamma r_1} - \frac{e}{r_1}$$

where in the last equation $N = 2\gamma^{3/2}/\sqrt{4\pi}$ has been substituted; this is the result of normalization of $\phi(r)$ to unity. Taking the potential due to the proton into account, the total electrostatic potential acting on the incident electron due to the perturbed hydrogen atom with the wave function $\phi(r)$ is given by

$$V_p = e\int(\frac{1}{r_1} - \frac{1}{r_{12}})|\phi(r_2)|^2d\vec{r}_2$$

$$= e(\gamma+\frac{1}{r_1})e^{-2\gamma r_1}$$

Appendix II

Evaluation of the integral:

$$\int_0^{\infty}\left[\frac{\alpha}{r(2r^3+\alpha)} - (\gamma + \frac{1}{r})e^{-2\gamma r}\right]dr = 0 \ .$$

Integrating the first term:

$$\int_0^{\infty} \frac{d}{r(2r^3+\alpha)}\, dr = \alpha\left[\frac{1}{3\alpha}\log\frac{r^3}{2r^3+\alpha}\right]_0^{\infty} = -\frac{1}{3}\log 2 - (\log r)_{r\to 0} + \frac{1}{3}\log\alpha \ .$$ [20]

Integrating the second term:

$$-\gamma\int_0^{\infty} e^{-2\gamma r}dr = \frac{-\gamma}{2\gamma} = -\frac{1}{2}$$

Integrating the third term:

$$-\int_0^{\infty}\frac{e^{-2\gamma r}}{r}\, dr = C + \log 2\gamma + (\log r)_{r\to 0}$$ [21]

where C = 0.577 is the Euler's constant. Adding the three terms

$$\frac{1}{3}\log\frac{\alpha}{2} - \frac{1}{2} + C + \log 2\gamma = 0 \ ,$$

or

$$\gamma = \frac{e^{1/2 - C}}{2(\alpha/2)^{1/3}} = \frac{0.583}{\alpha^{1/3}} \qquad .$$

Appendix III

Boundary Values of $U^{\pm}_{\ell_1}$ and $U^{\pm}_{\ell_2}$

By Taylor's expansion of $U^{\pm}_{\ell_1}$ about the origin,(4.5) takes the following from for small values of x:

$$(1) \qquad \left[\frac{d^2}{dx^2} + \frac{2\beta_o}{x}\right] U^{\pm}_{o_1}(x) = 0 \quad , \qquad \ell = 0$$

$$(2) \qquad \left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2}\right] U^{\pm}_{\ell_1}(x) = 0 \quad , \qquad \ell \neq 0 \ .$$

Substituting $U^{\pm}_{\ell_1}(x) = \sum\limits_{\nu=o}^{\infty} a_\nu x^\nu$ in (1) we get:

$$a_o = 0 \ , \qquad \sum_{\nu=1}^{\infty} a_\nu \left[\nu(\nu-1)x^{\nu-2} + 2\beta_o x^{\nu-1}\right] = 0 \ .$$

This indicial equation is satisfied if

$$a_{\nu+1} \cdot \nu(\nu-1) + 2\beta_o a_\nu = 0 \ ,$$

whence

$$a_{\nu+1} = \frac{2\beta_o}{\nu(\nu-1)} a_\nu \ .$$

Then all the a_ν are finite, and

$$(3) \qquad U^{\pm}_{o_1}(x) \underset{x \to o}{=} a_1 x \ .$$

Substitution of the same expansion into (2) results in

$$a_o = a_1 = 0 \ , \qquad \sum_{\nu=2}^{\infty} a_\nu \left[\nu(\nu-1)x^{\nu-2} - \ell(\ell+1)x^{\nu-2}\right] = 0$$

with $\nu = \ell + 1$ and

$$(4) \qquad U^{\pm}_{\ell_1}(x) \underset{x \to o}{=} a_{\ell+1} x^{\ell+1} \ .$$

It is seen that (4) includes (3) as well and then is valid for all values of ℓ.

To find the boundary value of $U^{\pm}_{\ell_2}$ we use again the Taylor expansion of $U^{\pm}_{\ell_2}$ in (4.6). For small values of x this equation reduces to

$$(5) \qquad \left[\frac{d^2}{dx^2} + \frac{2\beta_o}{x}\right] U^{\pm}_{o_2}(x) \mp \frac{8\beta_o\beta^3}{2\ell+1}\, x^{\ell+1} = 0\,, \qquad \ell = 0$$

$$(6) \qquad \left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2}\right] U^{\pm}_{\ell_2}(x) \mp \frac{8\beta_o\beta^3}{2\ell+1}\, x^{\ell+1} = 0\,, \quad \ell \neq 0\,.$$

The homogeneous solution of (5) and (6) are the same as (1) and (2). We only need the inhomogeneous solution of (5) and (6) to satisfy the boundary values of $U^{\pm}_{\ell}$. Substituting the expansion $U^{\pm}_{\ell_2}(x) = \sum_{\nu=o}^{\infty} a_\nu x^\nu$ in (6) we get

$$a_o = a_1 = 0, \quad \sum_{\nu=2}^{\infty} a_\nu \left[\nu(\nu-1) - \ell(\ell+1)\right] x^{\nu-2} \mp \frac{8\beta_o\beta^3}{2\,\ell+1}\, x^{\ell+1} = 0, \ \ell \neq 0\,.$$

This equation can be satisfied if $\nu = \ell+3$, and from this,

$$a_\nu = \frac{\pm 8\beta_o\beta^3}{(2\ell+1)\left[(\ell+3)(\ell+2) - \ell(\ell+1)\right]} = \frac{\pm 8\beta_o\beta^3}{2(2\ell+1)(2\ell+3)}\,.$$

Therefore

$$(7) \qquad U^{\pm}_{\ell_2}(x) \underset{x\to o}{=} \frac{\pm 8\beta_o\beta^3}{2(2\ell+1)(2\ell+3)}\, x^{\ell+3}\,.$$

From (4) and (7) we see that

$$U^{\pm}_{\ell}(x) = U^{\pm}_{\ell_1}(x) + C^{\pm}_{\ell}\, U^{\pm}_{\ell_2}(x) \underset{x\to o}{=} a_{\ell+1} x^{\ell+1}\,,$$

as it can also be inferred from the expansion of $U^{\pm}_{\ell}(x)$ in (4.3).

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